Theory of Spike Spiral Waves in a Reaction-Diffusion System

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We discovered a new type of spiral wave solutions in reaction-diffusion systems — spike spiral wave, which significantly differs from spiral waves observed in FitzHugh-Nagumo-type models. We present an asymptotic theory of these waves in Gray-Scott model. We derive the kinematic relations describing the shape of this spiral and find the dependence of its main parameters on the control parameters. The theory does not rely on the specific features of Gray-Scott model and thus is expected to be applicable to a broad range of reaction-diffusion systems.

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Formation of rotating spiral waves (rotors) is one of the most vivid and ubiquitous phenomena of nonlinear physics [1–11]. These waves are observed in nonlinear optical media [12], chemical reactions of Belousov-Zhabotinsky type, catalytic reactions on crystal surfaces [5–7], and in a variety of biological systems: social amoebae Dictyostelium discoideum [13], Xenopus oocytes [14], chicken retina [15], and the heart of animals and man, where the formation of spiral waves is responsible for cardiac arrythmias and the life-threatening condition of ventricular fibrillation [1,11].

A generic model used to describe spiral waves is a pair of reaction-diffusion equations of activator-inhibitor type [1–10]

$$\tau_\theta \frac{\partial \theta}{\partial t} = l^2 \Delta \theta - q(\theta, \eta, A), \quad (1)$$

$$\tau_\eta \frac{\partial \eta}{\partial t} = L^2 \Delta \eta - Q(\theta, \eta, A), \quad (2)$$

where θ is the activator, i.e., the variable with respect to which there is a positive feedback; η is the inhibitor, i.e., the variable with respect to which there is a negative feedback and which controls activator's growth; q and Q are certain nonlinear functions representing the activation and the inhibition processes; l and L are the characteristic length scales, and τ_θ and τ_η are the characteristic time scales of the activator and the inhibitor, respectively; and A is the bifurcation parameter. A considerable amount of studies was done on the excitable systems with FitzHugh-Nagumo-type kinetics (N-systems) (see, for example, [1–8] and references therein). These systems are described by Eqs. (1) and (2) with $L = 0$, and the nonlinearity in q such that the nullcline of Eq. (1) is N- or inverted N-shaped. Theory of the spiral waves in N-systems with $\alpha = \tau_\theta/\tau_\eta \ll 1$ was recently developed by Karma [16,17].

The existence of spiral waves in excitable N-systems is due to the ability of such systems to sustain traveling waves, the simplest of which is a solitary wave — traveling autosoliton (AS) [1–10]. In N-systems the equation $q(\theta, \eta, A) = 0$ has three roots: θ_{i1}, θ_{i2}, and θ_{i3}, for fixed A and $\eta = \eta_i$. For $\alpha \ll 1$ an AS consists of a front, which is a wave of switching from the stable homogeneous state $\theta = \theta_h$ and $\eta = \eta_h$ to the state with $\theta = \theta_{\max}$ ($\theta_h = \theta_{i1}$ and $\theta_{\max} = \theta_{i3}$ for $\eta_i = \eta_h$) whose width is of order l, and a back of width of order l that follows the front some distance $w \gg l$ behind the front. Thus, in the AS the distribution of θ is a broad pulse, while the value of η slowly varies from $\eta = \eta_h$ to some value $\eta = \eta_m$ in the back of the pulse, and then slowly recovers from η_m to η_h behind it. In the limit $\alpha \to 0$ the amplitude of the wave (the value of $\theta_{\max}$) becomes independent of α and the speed c does not exceed the value of order l/τ_θ, with both $\theta_{\max}$ and c determined only by the nonlinearity in q.

At the same time, many excitable systems are described by Eqs. (1) and (2) in which the nullcline of Eq. (1) is Λ- or V-shaped. Examples of such Λ-systems are the well-known Brusselator and Gray-Scott models of autocatalytic reactions and an example of a V-system is the Gierer-Meinhardt model of morphogenesis [9]. Recently, we showed for the excitable Brusselator [18] and Gray-Scott model [19] that they are also capable of propagating traveling waves — traveling spike AS. The properties of these AS are essentially different from those in N-systems. The distribution of θ in an AS has the form of a narrow spike whose amplitude grows as α decreases and can become huge as $\alpha \to 0$. In contrast to N-systems, in the spike η varies abruptly and then slowly recovers back to η_h far behind the spike. The speed of such an AS is always greater than l/τ_θ and goes to infinity as $\alpha \to 0$. Also, it is important to emphasize that in an AS the front

and the back are not separated by a large distance, as in N-systems. In this Letter we will show that in excitable Λ- or V-systems it may also be possible to excite steadily rotating spiral waves and develop a theory of such waves in the case $\alpha \ll 1$.

To be specific, we will consider excitable ($L = 0$) Gray-Scott model, which is described by the following equations [20]

$$\frac{\partial \theta}{\partial t} = \Delta\theta + A\theta^2\eta - \theta, \tag{3}$$

$$\alpha^{-1}\frac{\partial \eta}{\partial t} = -\theta^2\eta + 1 - \eta, \tag{4}$$

where we chose l and τ_θ as the units of time and space, respectively. Recently, we showed numerically that a steadily rotating spiral waves may be excited in this model at sufficiently small α [19]. From these simulations one can see that the spiral wave is a steadily rotating slightly curved sharp spike front of width of order 1 which in the cross-section looks like a periodic traveling wave train (sufficiently far from the core). We would like to emphasize that it is this kind of the concentration profiles that is experimentally observed in Belousov-Zhabotinsky reaction [21,22].

Let us derive the equation of motion for the traveling sharp front in Gray-Scott model with $\alpha \ll 1$. Since η varies slowly outside the front, it can be replaced by a constant value $\eta = \eta_i$ ahead of the front. Let us introduce self-similar variable $z = \rho - ct$, where ρ is the coordinate along the normal direction to the front. For definiteness we will assume that $c > 0$, what means that the front is moving in the $+z$ direction. In the sharp front the value of θ is large [19], so one can neglect the last two terms in Eq. (4). Therefore, in the presence of small curvature K Eqs. (3) and (4) can be written as

$$\frac{d^2\theta}{dz^2} + (c + K)\frac{d\theta}{dz} + A\theta^2\eta - \theta = 0, \tag{5}$$

$$\alpha^{-1}c\frac{d\eta}{dz} - \theta^2\eta = 0. \tag{6}$$

These equations have to be supplemented by the boundary conditions $\theta(\pm\infty) = 0$ and $\eta(+\infty) = \eta_i$, where the infinity actually means sufficiently far ahead of the front compared to the front thickness.

Let us introduce new variables

$$\tilde{\theta} = \alpha^{1/2}\theta\left(\frac{c + K}{c}\right)^{1/2}, \quad \tilde{\eta} = \frac{\eta}{\eta_i}, \tag{7}$$

and the following quantities

$$\tilde{A} = A\alpha^{-1/2}\eta_i\left(\frac{c}{c + K}\right)^{1/2}, \quad \tilde{c} = c + K. \tag{8}$$

In these variables Eqs. (5) and (6) become

$$\frac{d^2\tilde{\theta}}{dz^2} + \tilde{c}\frac{d\tilde{\theta}}{dz} + \tilde{A}\tilde{\theta}^2\tilde{\eta} - \tilde{\theta} = 0, \tag{9}$$

$$\tilde{c}\frac{d\tilde{\eta}}{dz} - \tilde{\theta}^2\tilde{\eta} = 0, \tag{10}$$

with the boundary condition $\tilde{\eta}(+\infty) = 1$. Observe that all α-, A- and η_i-dependences now enter only via the parameter $\tilde{A}$.

Equations (9) and (10) have been analyzed by us in [19]. There we showed that these equations indeed admit solutions in the form of a traveling spike. In the spike $\tilde{\eta}$ varies from $\tilde{\eta} = 1$ at $z = +\infty$ (ahead of the front) to some $\tilde{\eta} = \tilde{\eta}_{\min}$ at $z = -\infty$ (behind the front). The value of $\tilde{\theta} \sim 1$ in the spike, so in the original variables we indeed have $\theta \sim \alpha^{-1/2} \gg 1$ [see Eq. (7)]. The speed of the front $\tilde{c}$ as a function of $\tilde{A}$ obtained from the numerical solution of Eqs. (9) and (10) is presented in Fig. 1 [19]. One can see that this solution exists only for $\tilde{A} > \tilde{A}_b$, and its speed is always greater than $c = c_{\min}$, where

$$\tilde{A}_b = 3.76, \quad c_{\min} = 1.5 \tag{11}$$

The analysis of Eqs. (9) and (10) also shows that $\tilde{\eta}_{\min} = \tilde{\eta}^b_{\min} = 0.05$ at $\tilde{A} = \tilde{A}_b$ and rapidly decreases as $\tilde{A}$ increases [19].

From Eq. (8) immediately follows that for small K the correction δc to the velocity c due to curvature is

$$\delta c = -K\left(1 + \frac{\tilde{A}}{2\tilde{c}}\frac{d\tilde{c}}{d\tilde{A}}\right), \tag{12}$$

where in the right-hand side $\tilde{A}$, $\tilde{c}$, and $d\tilde{c}/d\tilde{A}$ are evaluated at $K = 0$. Also, as we showed in [19], for $\tilde{A}$ not in the immediate vicinity of $\tilde{A}_b$ with good accuracy $\tilde{c} = 0.86\tilde{A}$ and $\tilde{\eta}_{\min} = 0$. Then, going back to the original variables, we may write

$$c = c_\infty - aK, \tag{13}$$

where

$$c_\infty = 0.86A\alpha^{-1/2}\eta_i, \quad a = \frac{3}{2}. \tag{14}$$

Behind the sharp front the value of η drops from η_i to $\eta_{\min}$ and θ goes exponentially to zero [19]. On the much longer time scale α^{-1} the value of η recovers from $\eta_{\min}$ according to Eq. (4), in which outside of the front the term $-\theta^2\eta$ can be neglected. From this we obtain that after the front passed a point x at time $t_i = t_i(x)$ we have

$$\eta(x, t) = 1 - [1 - \eta_{\min}(t_i)]e^{-\alpha(t - t_i)}, \tag{15}$$

where $\eta_{\min} = \eta_i\tilde{\eta}_{\min}$. In a steadily rotating spiral wave we must have $\eta(x, t_i + T) = \eta_i(t_i) = \text{const}$, where $T = 2\pi/\omega$ and ω is the angular frequency of the rotation of the spiral. Therefore, the spiral should be described by Eq. (13) with $c_\infty = \text{const}$, which is in turn related to ω. This equation was first analyzed by Burton, Cabrera, and

Frank (BCF) for growth of screw dislocations on crystal surfaces [23] (see also [8]). They calculated the shape of the spiral and its frequency in the case when the tip of the spiral is at rest. Applying their results to Eq. (14), we obtain $\omega = 0.16\alpha^{-1}A^2\eta_i^2$, where for simplicity we used the expressions in Eq. (14) and put $\eta_{\min} = 0$. Since $A\eta_i \gtrsim \alpha^{1/2}$ in order for the front to be able to propagate, we must have $\omega \gtrsim 1$, so one can expand the exponential in Eq. (15), and obtain $\eta_i = 3.4\alpha^{2/3}A^{-2/3}$ and $\omega = 1.8\alpha^{1/3}A^{2/3}$. The spatial step h of the spiral far from the core will be $h = 10\alpha^{-1/6}A^{-1/3}$. Notice that a similar method was recently used to analyze asymptotically the spiral waves in N-systems [16,17].

Comparing the results obtained above with Eq. (11), one can see that in order for the solution in the form of the traveling front to exist, one should have $A \gtrsim \alpha^{-1/2} \gg 1$. On the other hand, for $A \gg \alpha^{-1/2}$ we have $\omega \gg 1$, so θ will not have enough time to decay behind the wave front. This means that this kind of spiral wave may exist only at $A \sim \alpha^{-1/2}$. Notice that according to Eq. (14) we have $c_\infty \sim 1$ and $h \sim 1$ for these values of A, so the formulas obtained above for the frequency of the spiral should only be correct qualitatively.

These facts may seem rather surprising since they predict that the spiral waves should exist only in a narrow range of the values of A far from the excitability threshold $A = A_{bT} = 3.76\alpha^{1/2}$, which is obtained from Eq. (11) for $\eta_i = \eta_h = 1$ [19]. Also, numerical simulations show that spiral waves exist in a wide range of the values of A. What we will show below is that the spiral waves actually exist for all values of $A_b < A \lesssim \alpha^{-1/2}$.

The thing is that in addition to the spiral wave solution whose tip is at rest, there may also be a solution whose tip moves along a circle of some radius R, which can be large for $A\alpha^{1/2} \ll 1$. The reason the front will not propagate inside the circle is that the tip is right at the propagation threshold. This means that for $A \ll \alpha^{-1/2}$ we have $\eta_i = \eta_i^b = 3.76\alpha^{1/2}A^{-1}$ in the limit $\alpha \to 0$ (for $R \gg 1$ the corrections due to curvature can be neglected), so the frequency ω is determined by Eq. (15) with $\eta_i = \eta_i^b$. In particular, for $\alpha^{1/2} \ll A \ll \alpha^{-1/2}$ we can expand the exponential and obtain asymptotically

$$\omega = 1.76\alpha^{1/2}A. \tag{16}$$

This equation shows that the value of ω lies in the range $\alpha \lesssim \omega \lesssim 1$, as should be expected. For large values of R the speed of the front far away from the core should only slightly exceed $c_{\min}$, so the step of the spiral will be $h = 5.4\alpha^{-1/2}A^{-1}$. Note, however, that because of the closeness to the threshold point $\tilde{A} = \tilde{A}_b$ the expansion in Eq. (12) is no longer justified and therefore the BCF theory, as well as Eq. (13), is not applicable to the spiral waves in this parameter range. This theory can be modified by noting that close to $\tilde{A}_b$ we have approximately

$$c = c_{\min} + b\left(\tilde{A} - \tilde{A}_b - \frac{\tilde{A}_b}{2c_{\min}}K\right)^{1/2}, \tag{17}$$

where b is a constant and the tilde quantities in the right-hand side are evaluated at $K = 0$. The analysis of Eqs. (9) and (10) shows that $b = 1.4$. Observe that this equation reduces to the form of Eq. (13) only very far from the core.

Following [23], we rewrite Eq. (17) for the steadily rotating spiral in terms of the angle ϕ between the tangent vector to the front and the radius vector as a function of the distance r to the origin. A straightforward calculation shows that in these variables Eq. (17) becomes

$$\begin{aligned}\frac{d\phi}{dr} = {} & -\frac{1}{r}\tan\phi \\ & + \frac{2c_{\min}}{\tilde{A}_b b^2 \cos\phi}\left[b^2(\tilde{A} - \tilde{A}_b) - (c_{\min} - \omega r\cos\phi)^2\right],\end{aligned} \tag{18}$$

with the boundary conditions $\phi(+\infty) = \pi/2$ [23] and $\phi(R) = 0$. The latter condition says that at its tip the front is normal to the circle along which it rotates, what follows from the physical considerations. Since the front at $r = R$ is at its propagation threshold, its normal velocity there should be equal to $c_{\min}$. This, together with the boundary condition at $r = R$ immediately gives us $R = c_{\min}/\omega$. Knowing the value of R, one can then calculate $\tilde{A} - \tilde{A}_b$ and find the value of ω for which it agrees with Eq. (15). This will determine a unique value of ω. Numerical solution of Eq. (18) shows that for $\omega \ll 1$ we have $\tilde{A} - \tilde{A}_b \ll 1$, so Eq. (16) should indeed be recovered in the limit $\alpha \to 0$ with $\alpha^{1/2} \ll A \ll \alpha^{-1/2}$, and the spiral wave solution is an involute of a circle of radius R.

The solution of Eq. (18) for $\omega = 0.29$ is presented in Fig. 2. For this value of ω we found $\tilde{A} - \tilde{A}_b = 0.34$, which gives $\eta_i = 0.86$, within 4% in agreement with Eq. (15). Comparing these quantities with the results of the numerical simulations of Eqs. (3) and (4) for $\alpha = 0.1$ and $A = 1.5$, in which this value of ω was observed, we find that the value of η_i agrees with the predicted one within 3% accuracy. The speed $c_\infty = 2.3$ obtained from Eq. (17) also agrees with that observed numerically within a few per cent accuracy.

This agreement is quite remarkable considering the fact that at these parameters the spiral wave already underwent meandering instability. In fact, according to our analysis, steady rotation of the spiral requires fine-tuning of the value of η_i at the tip of the spiral. Note that the tip of the spiral is not described by the interfacial equations derived above and thus is a rather singular object capable of sudden movements on the smallest length scale. Thus, it is natural to expect that the tip trajectory in a meandering spiral may be rather abrupt. Notice that similar situation is observed in the simulations of models of cardiac tissue (see, for example, [24]).

In conclusion, we developed a theory of spike spiral waves in Gray-Scott model. Spike traveling waves are observed in a variety of excitable systems including nerve and cardiac tissue. Even though we performed an analysis of a concrete system, Eqs. (17) and (18) have general

character and thus are expected to apply to other Λ- and V-systems (see also [9,10]) and other excitable systems of different nature in which spike traveling waves are observed. Also, such waves can be expected in combustion systems and Belousov-Zhabotinsky reaction in continuous flow reactors. The thing is that although in Eqs. (1) and (2) describing these systems the activator nullcline may formally be N-shaped, for typical parameters the value of $\theta_{\max}$ may be several orders of magnitude greater than θ_h, so the system effectively behaves as a Λ- or V-system. In particular, this is true for the models of systems with uniformly generated combustion material [9,10] and the two-parameter version of Oregonator [25].

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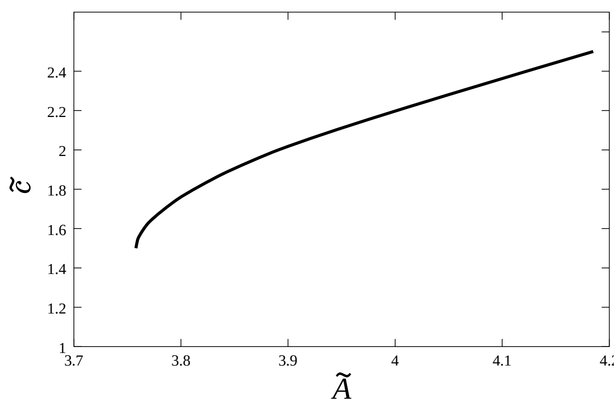

FIG. 1. Dependence $\tilde{c}(\tilde{A})$ obtained from the numerical solution of Eqs. (9) and (10).

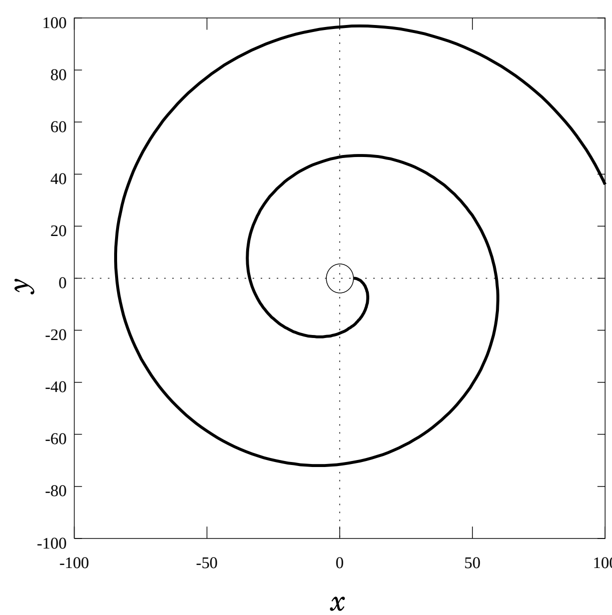

FIG. 2. Steadily rotating spiral wave. Results of the numerical solution of Eq. (18) with $\omega = 0.29$ and $\tilde{A} - \tilde{A}_b = 0.34$. The circle shows the core of the spiral.